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Editorial

Protein Conformational Computations-special issue of *Polymer*

Application of computations to proteins is an extremely active field of which many of the readers of *Polymer* may not be aware. While polymer computations have had major impacts on the polymer field, it is likely that protein computations will eventually have a significantly larger effect on molecular biology. There are several reasons for this:

1. Protein structures are extremely large and complex and hence their comprehension is difficult—computations assist in this direction.
2. It is a growing field and will continue to grow for a long time. Many functional biological structures are extremely large, and imaging is developing rapidly that will give us many more structural details.
3. Better understanding of biological function at the molecular level will yield huge benefits for health, nutrition and economics.

We intend the collection of papers for this special issue of Polymer to provide a snapshot of some of the excitement in this field at present. In this issue we have a number of articles on coarse-grained supra-atomic approaches to protein structure (1-3). In many ways these approaches resemble the old ways in which equivalent chain models were developed to describe polymers. The folding–unfolding transition is an extremely important and popular area to understand, both in equilibrium and kinetic terms, and this work is well represented here (4-7). Empirical approaches to describe the observed interactions for use with the coarse-grained protein models have been popular and these resemble the empirical evaluations of interactions in polymer chains pursued by Scheraga, Flory and others (8-11). Rubber elasticity is finding important applications in treating deformations of coarse-grained protein structures (12-14). Generally there is also a class of problems for characterizing sets of protein conformations that in some ways closely resembles polymer conformational characterization problems (15-16).

Proteins do not resemble usual polymers because they normally have quite unique folded forms, and this leads to new classes of computational approaches, such as threading where new protein sequences are mounted upon the known protein structures (17), and coarse-grained interaction models are used for their evaluations. The designability of a given structure relates to finding the sequences for which a given structure is appropriate (18). Protein compactness means that new methods are required for the conformation generations (19-20).

We do hope you enjoy reading this special issue of Polymer, and thank the editors for inviting us to address their special audience. We would, especially like to thank all contributors for interesting papers submitted to the special issue of Polymer.

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